

Heptane

C7H16								
pi	nu 0	e	h bar	m sub e	a0	c	mp	
	3.1415927E+00	1.2566371E-06	1.6021892E-19	1.0545888E-34	9.1095345E-31	5.2917706E-11	2.9979246E+08	1.6726486E-27
	epsilon 0	uB	eV/cm^-1		aH		md	
		8.85E-12	9.27E-24	0.000123985	5.29465E-11		3.3435860E-27	
cm-1/eV								
	1.239810E-04							
kcal/mole/eV		Total Bond Energy CH3 (eV)						
		12.49186						
	4.336340E-02							
kJ/mole/eV		Total Bond Energy CH2 (eV)						
		7.83016						
	0.010364101							
C		Total Bond Energy C-C (eV)						
		4.32754						
	716.68							
	7.42774							
H		Heptane Total E (eV)						
		90.09976						
	217.998							
	2.259353							
heptane		Exp Heptane Total E (eV)						
		90.08817						
	-187.6							
	-1.9443							
		Rel. Error						
		-0.000128671						
	88.14386285							
total bond energy								
	90.08817							